Electronic Supplementary Information

for

Vinylpyrroles: Solid-state structures and aggregation-induced emission properties

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Crystallographic data for 1 and 2

Table S1. Crystallographic data for **1** and **2**

	Compound **1**	Compound **2**
Empirical formula	$C_{20}H_{25}NO_8$	$C_{20}H_{25}N_3O_7$
Formula weight	407.42	419.44
Crystal size / mm^3	0.48 × 0.28 × 0.20	0.30 × 0.30 × 0.15
Crystal system	Monoclinic	Monoclinic
Space group	*C*2/c	$P2_1/c$
a / Å	20.82(11)	17.799(2)
b / Å	12.78(6)	5.2201(7)
c / Å	17.52(9)	21.974(3)
β / °	98.80(4)	101.833(13)
Volume / $Å^3$	4605(41)	1998.3(5)
Z	8	4
Wavelength / nm	0.71073	0.71073
Temperature / K	296	123
Density / $g·cm^{-3}$	1.175	1.3941
Absorption coefficient / mm	0.091	0.106
F(000)	1729	888
Reflections collected	10080	10080
Data/restraints/parameters	3367/36/267	4094/36/276
Goodness of fit	1.05	1.11
$R1$ [$I > 2\sigma(I)$]	0.0767	0.0888
*wR*2 (all data)	0.2312[(a)]	0.2756[(b)]
Largest diff. peak and hole, e· $Å^{-3}$	0.3233, −0.3556	0.6459, −0.5536

(a) $w = 1/[\sigma^2(F_o^2)+(0.1437P)^2]$, where $P = (F_o^2+2F_c^2)/3$,

(b) $w = 1/[\sigma^2(F_o^2)+(0.1061P)^2+2.3620P]$, where $P = (F_o^2+2F_c^2)/3$.

Table S2. Bond lengths and angles for **1**

Atom-Atom	Bond lengths [Å]	Atom-Atom	Bond lengths [Å]
O1–C7	1.255(6)	C1–C5	1.462(7)
O2–C8	1.231(6)	C2–C3	1.457(7)
O3–C7	1.382(6)	C2–C9	1.514(7)
O3–C11	1.489(9)	C3–C4	1.427(8)
O4–C8	1.393(7)	C3–C14	1.545(7)
O4–C11	1.469(7)	C4–C10	1.515(7)
O5–C9	1.239(7)	C5–C6	1.399(7)
O6–C9	1.359(7)	C6–C7	1.507(8)
O6–C17	1.488(7)	C6–C8	1.523(7)
O7–C10	1.237(6)	C11–C12	1.543(8)
O8–C10	1.373(8)	C11–C13	1.529(8)
O8–C19	1.485(6)	C14–C15	1.564(8)
N1–C1	1.388(6)	C15–C16	1.554(8)
N1–C4	1.387(6)	C17–C18	1.486(9)
C1–C2	1.459(8)	C19–C20	1.517(9)
Atom-Atom-Atom	Bond angles [°]	Atom-Atom-Atom	Bond angles [°]
C11–O3–C7	118.8(3)	C6–C7–O1	126.8(3)
C11–O4–C8	117.4(3)	C6–C7–O3	116.3(3)
C17–O6–C9	117.4(4)	O4–C8–O2	118.1(3)
C19–O8–C10	117.5(3)	C6–C8–O2	125.1(4)
C4–N1–C1	111.4(3)	C6–C8–O4	116.7(3)
C2–C1–N1	106.0(3)	O6–C9–O5	122.6(4)
C5–C1–N1	125.1(3)	C2–C9–O5	125.2(4)
C5–C1–C2	128.9(3)	C2–C9–O6	112.1(3)
C3–C2–C1	107.9(3)	O8–C10–O7	123.5(3)
C9–C2–C1	123.5(3)	C4–C10–O7	126.2(3)
C9–C2–C3	128.5(3)	C4–C10–O8	110.2(3)
C4–C3–C2	105.7(3)	O4–C11–O3	109.2(3)
C14–C3–C2	129.6(3)	C12–C11–O3	105.7(4)
C14–C3–C4	124.6(3)	C12–C11–O4	106.8(3)
C3–C4–N1	108.9(3)	C13–C11–O3	110.9(3)
C10–C4–N1	120.3(3)	C13–C11–O4	110.7(4)
C10–C4–C3	130.8(3)	C13–C11–C12	113.3(3)
C6–C5–C1	134.0(3)	C15–C14–C3	113.6(3)
C7–C6–C5	125.3(3)	C16–C15–C14	113.2(3)
C8–C6–C5	116.9(3)	C18–C17–O6	105.6(4)
C8–C6–C7	117.7(3)	C20–C19–O8	108.4(3)
O3–C7–O1	116.8(3)		

Table S3. Bond lengths and angles for **2**

Atom-Atom	Bond lengths [Å]	Atom-Atom	Bond lengths [Å]
O1–C7	1.228(5)	C6–C8	1.470(6)
O7–C11	1.320(5)	C6–C5	1.366(6)
O7–C19	1.463(5)	N1–C4	1.350(6)
O2–C8	1.235(5)	N1–C1	1.366(5)
O6–C10	1.327(6)	C11–C2	1.494(6)
O6–C17	1.474(5)	C4–C3	1.411(6)
O4–C10	1.211(5)	C4–C10	1.467(6)
O5–C11	1.206(5)	C2–C1	1.417(6)
O3–C9	1.189(6)	C2–C3	1.415(6)
N2–C9	1.407(6)	C12–C3	1.495(6)
N2–C8	1.366(6)	C12–C13	1.528(7)
N2–C16	1.471(6)	C19–C20	1.502(7)
N3–C9	1.387(6)	C1–C5	1.414(6)
N3–C7	1.389(6)	C13–C14	1.498(7)
N3–C15	1.465(5)	C18–C17	1.495(7)
Atom-Atom-Atom	Bond angles [°]	Atom-Atom-Atom	Bond angles [°]
C19–O7–C11	115.8(3)	C6–C7–O1	124.8(4)
C17–O6–C10	115.5(3)	C6–C7–N3	116.9(4)
C8–N2–C9	124.9(4)	C1–C2–C11	123.2(4)
C16–N2–C9	116.7(4)	C3–C2–C11	127.8(4)
C16–N2–C8	118.3(4)	C3–C2–C1	108.8(4)
C7–N3–C9	124.9(4)	C13–C12–C3	111.3(4)
C15–N3–C9	117.1(4)	C20–C19–O7	106.3(4)
C15–N3–C7	118.0(4)	N2–C8–O2	120.1(4)
N2–C9–O3	121.0(4)	C6–C8–O2	122.5(4)
N3–C9–O3	122.4(4)	C6–C8–N2	117.4(4)
N3–C9–N2	116.6(4)	C2–C1–N1	106.1(4)
C8–C6–C7	119.1(4)	C5–C1–N1	125.9(4)
C5–C6–C7	125.8(4)	C5–C1–C2	128.0(4)
C5–C6–C8	115.1(4)	C2–C3–C4	105.0(4)
C1–N1–C4	110.8(4)	C12–C3–C4	126.3(4)
O5–C11–O7	123.8(4)	C12–C3–C2	128.7(4)
C2–C11–O7	112.2(4)	O4–C10–O6	123.4(4)
C2–C11–O5	124.0(4)	C4–C10–O6	114.1(4)
C3–C4–N1	109.3(4)	C4–C10–O4	122.5(4)
C10–C4–N1	116.5(4)	C1–C5–C6	135.3(4)
C10–C4–C3	134.1(4)	C14–C13–C12	112.3(4)
N3–C7–O1	118.3(4)	C18–C17–O6	106.4(4)

Viscosity effects on the UV-vis and fluorescence spectra of 2

50 µL of a stock solution of **2** in CH_2Cl_2 with a concentration of 1.0×10^{-3} M was stored in glass tubes. After removal of the solvent, the residue was re-dissolved in 5 mL of methanol/glycerol solvents (100/0, 50/50, 40/60, 30/70, 20/80 and 10/90, *v*/*v*). UV-vis spectra (**Fig S1**) indicates there are no precipitates in all of the solutions. The fluorescence spectra were measured as prepared (**Fig S2**).

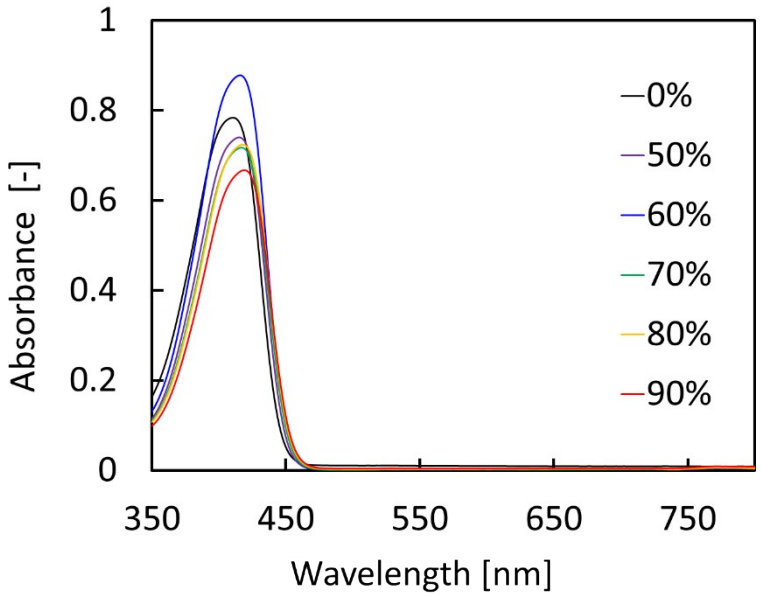


Fig S1. UV-vis spectra of **2** in methanol/glycerol solutions.

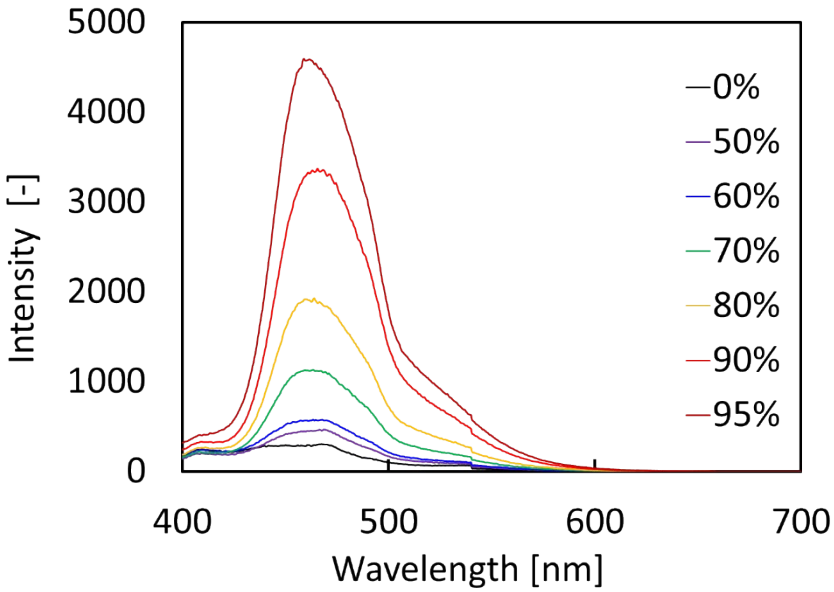


Fig S2. Fluorescence spectral change of **2** based on the glycerol fraction present in the methanol solution.

Solvent effects on the UV-vis and fluorescence spectra of 1 and 2

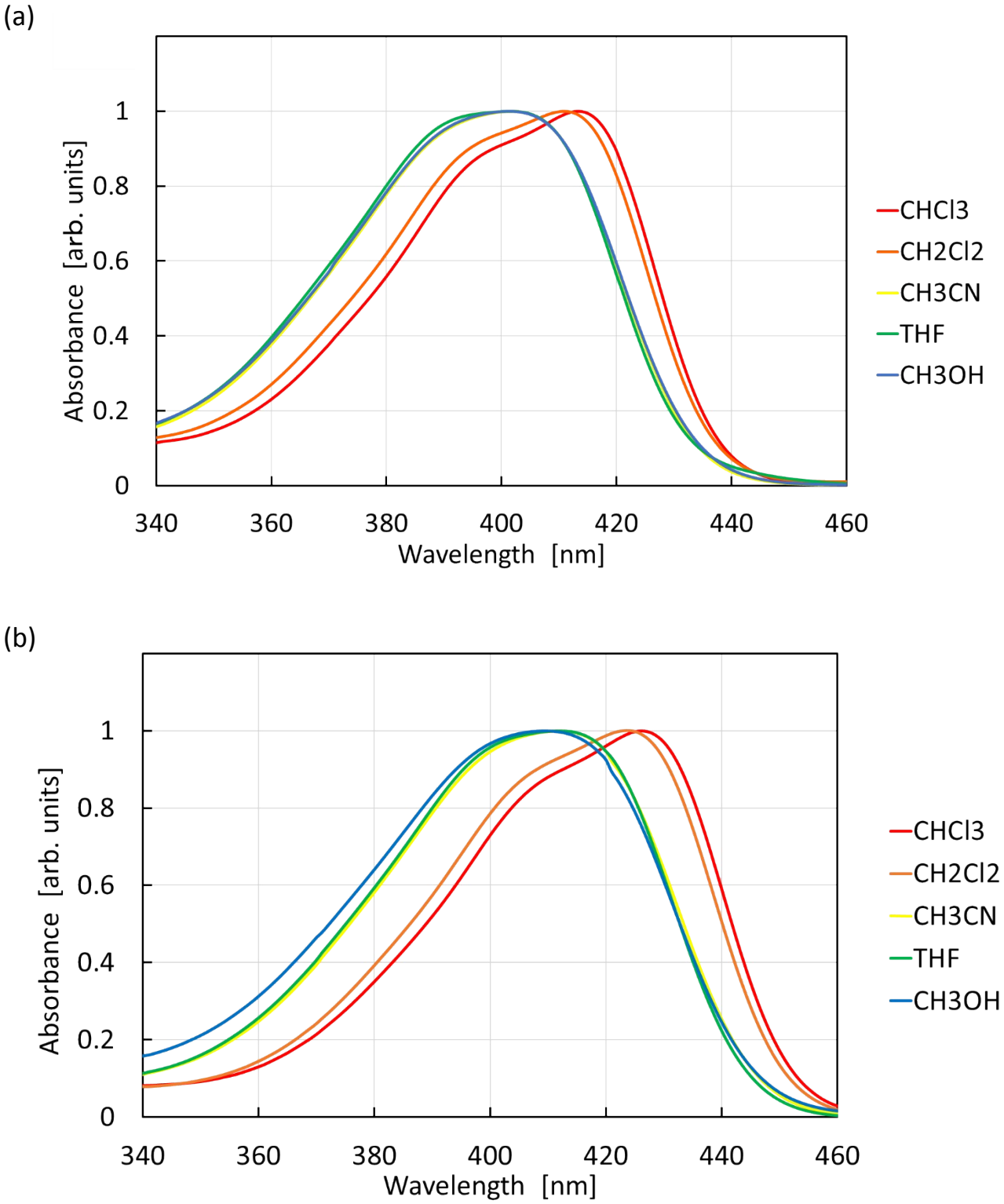
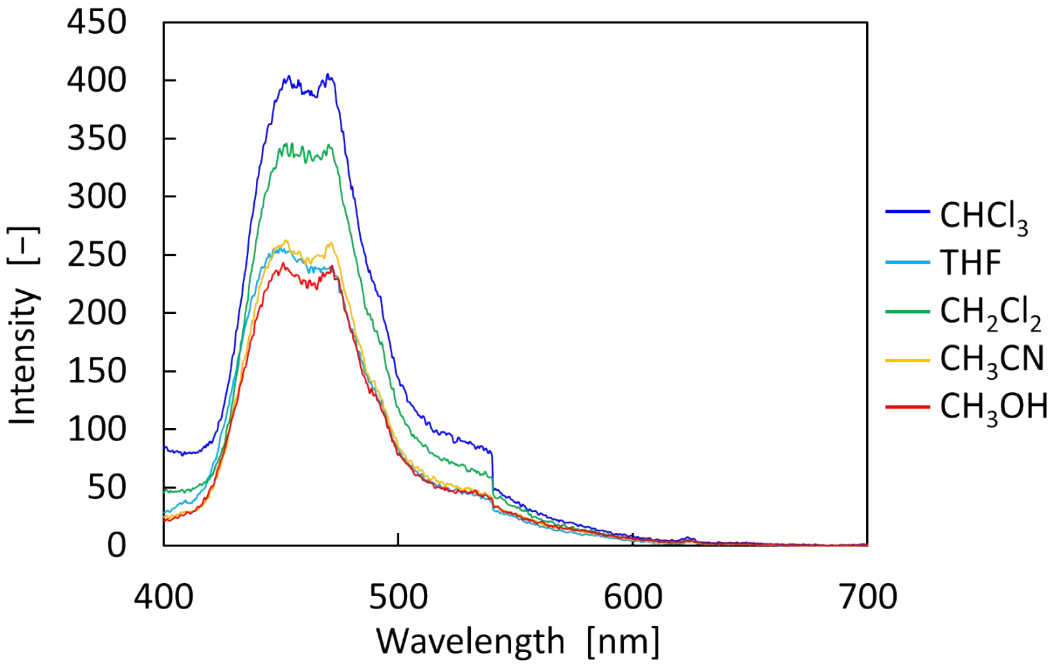


Fig S3. UV-vis absorption spectra for (a) **1** and (b) **2** in $CHCl_3$, CH_2Cl_2, CH_3CN, THF and CH_3OH.

(a)



(b)

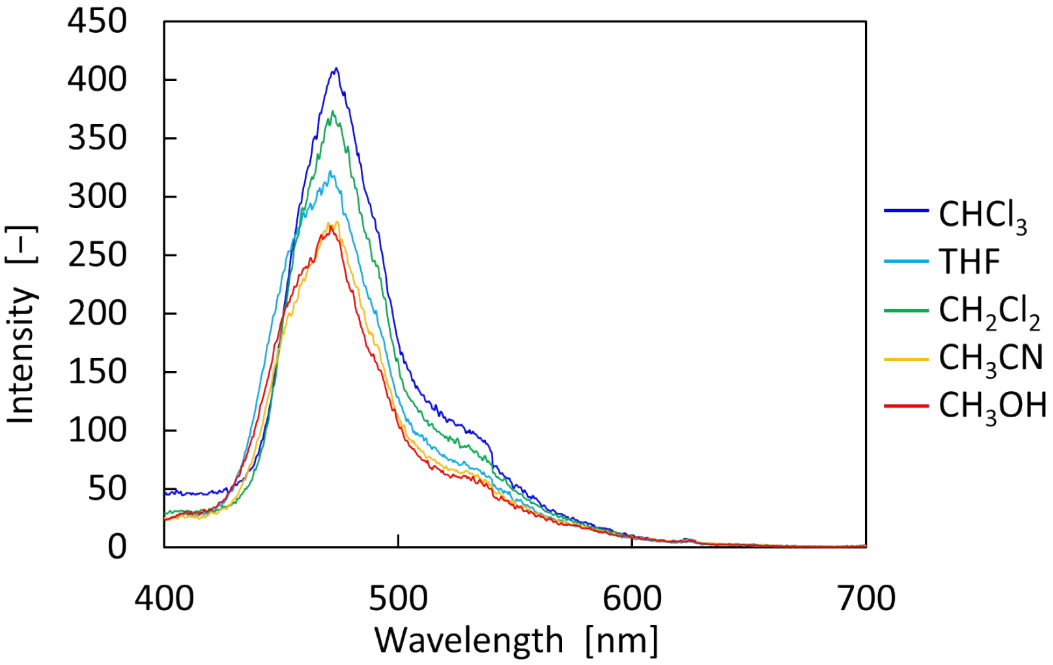
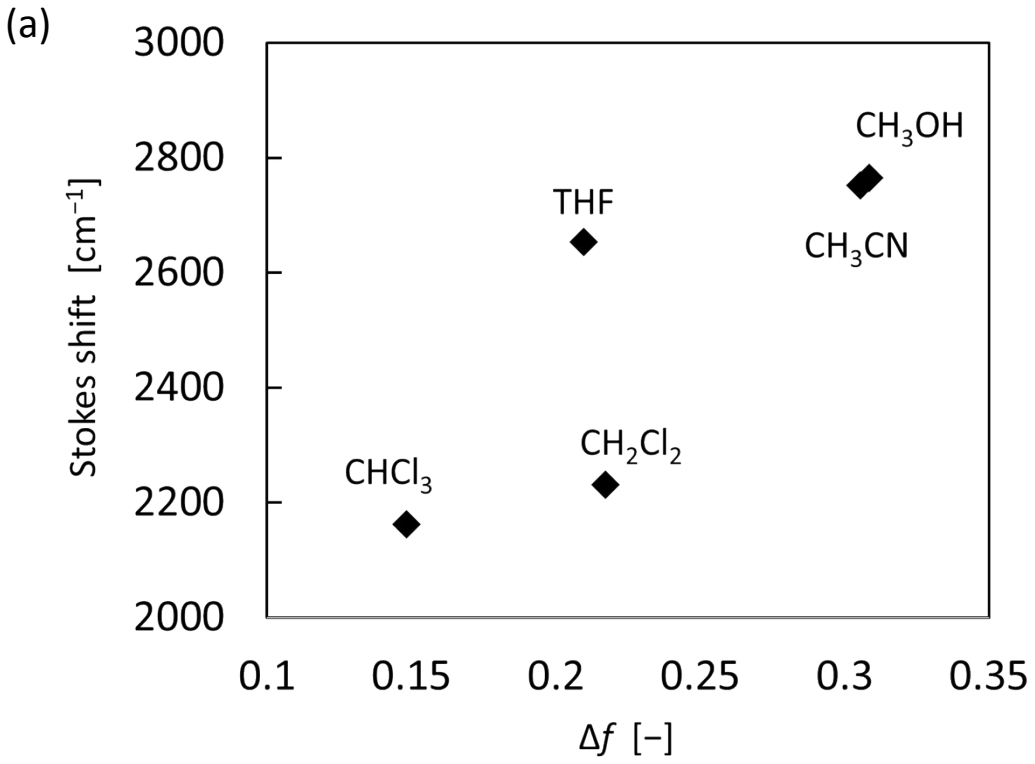


Fig S4. Fluorescence spectra for (a) **1** and (b) **2** in $CHCl_3$, CH_2Cl_2, CH_3CN, THF and CH_3OH.



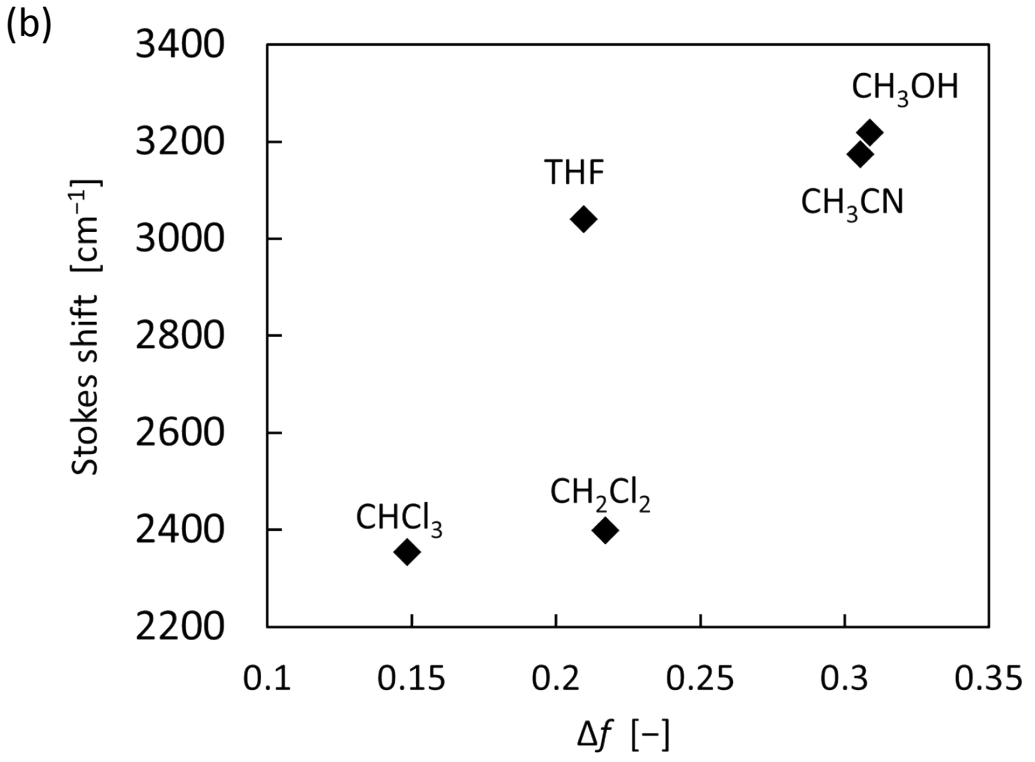


Fig S5. Mataga-Lippert plots for (a) **1** and (b) **2**. $\Delta f = (\varepsilon-1)/(2\varepsilon+1)-(n^2-1)/(2n^2+1)$.

^{1}H, ^{13}C NMR, ESI-MS, IR spectral data and elemental analysis for 1 and 2

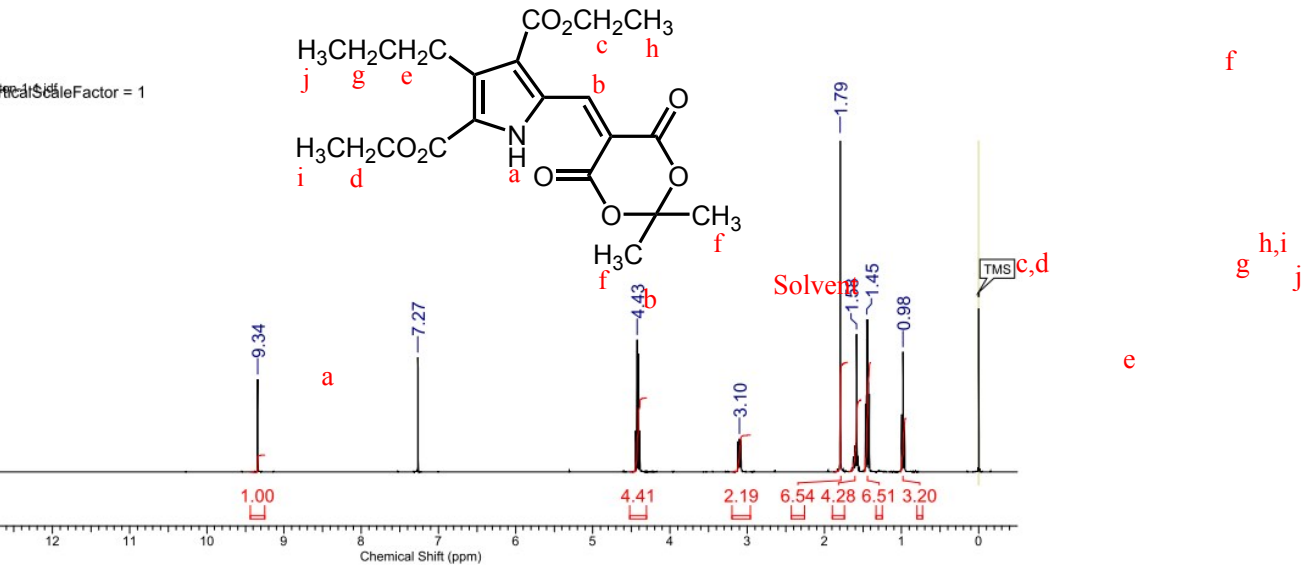
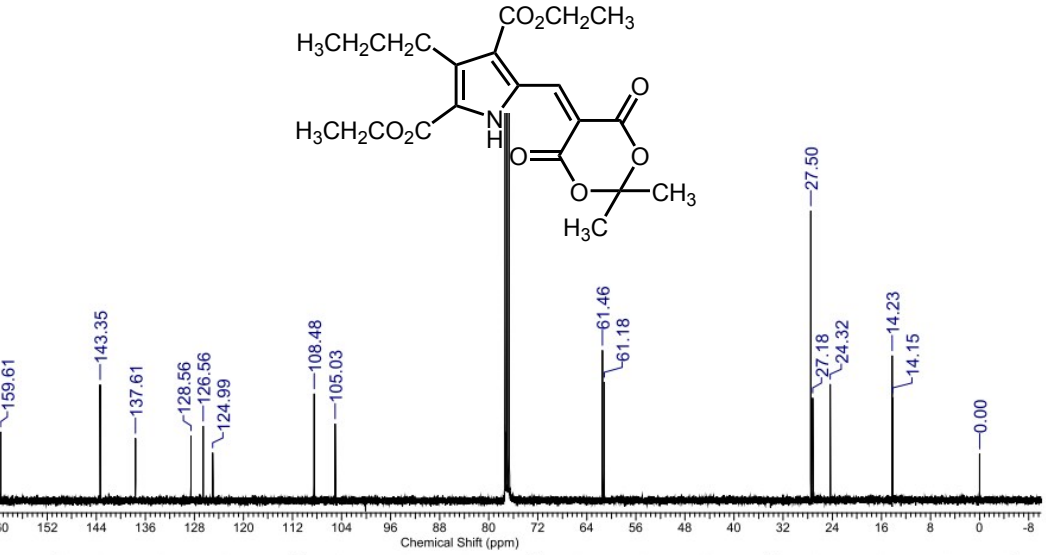


Fig S6. ^{1}H NMR spectrum of **1** in $CDCl_3$ at 25℃.



Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
0.0217	5	24.32	2445.0	0.0547	9	61.46	6178.0	0.0707	13	126.56	12722.2	0.0349	17	159.61	16045.0	0.0322
0.0482	6	27.18	2732.0	0.0483	10	105.03	10558.3	0.0360	14	128.56	12923.9	0.0304	18	162.82	16367.4	0.0204
0.0418	7	27.50	2764.1	0.1367	11	108.48	10905.1	0.0502	15	137.61	13833.8	0.0292	19	163.60	16445.9	0.0181
0.0683	8	61.18	6150.1	0.0556	12	124.99	12564.4	0.0223	16	143.35	14410.2	0.0545	20	163.75	16461.1	0.0247

Fig S7. ^{13}C NMR spectrum of **1** in $CDCl_3$ at 25℃.

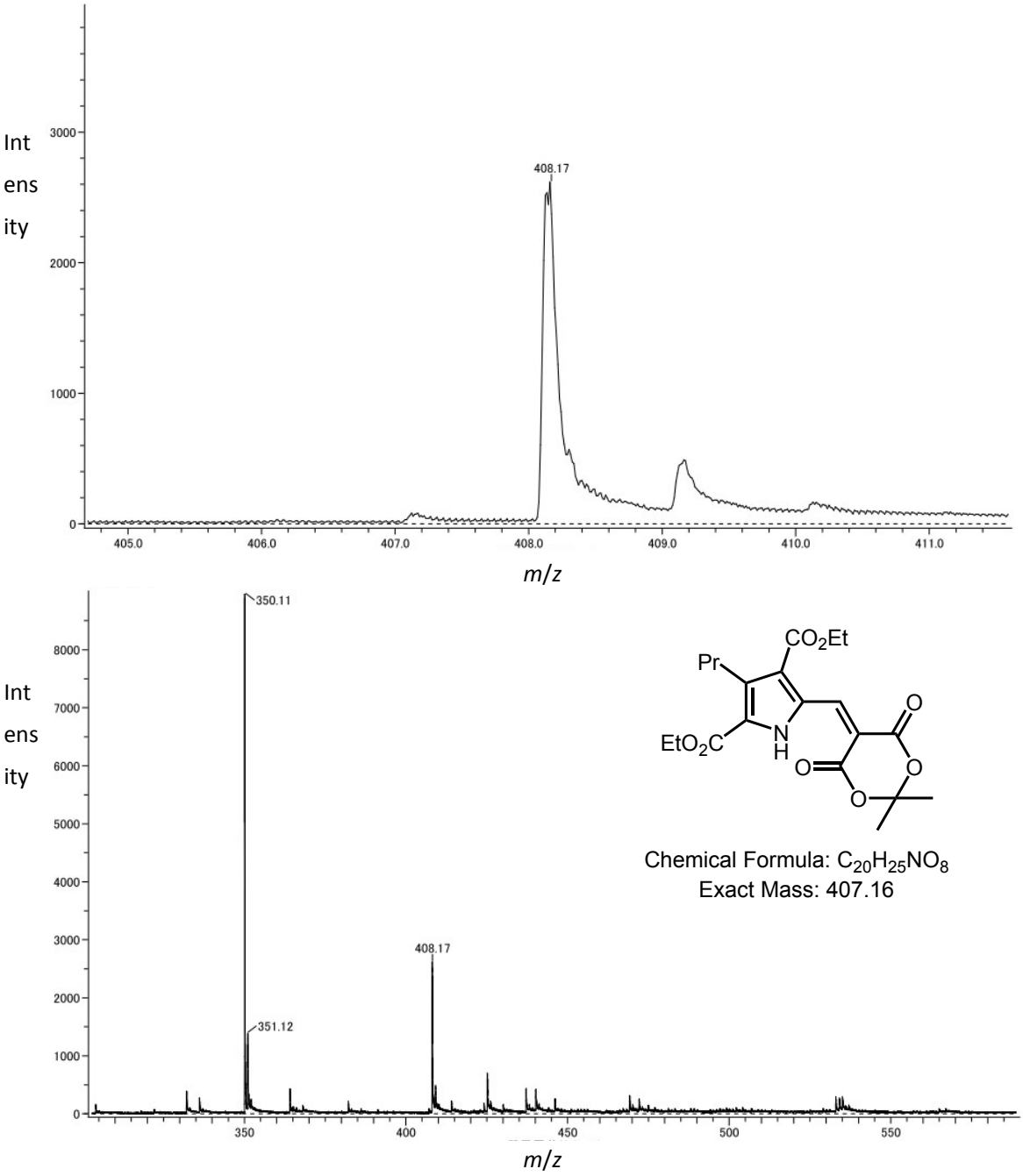


Fig S8. ESI-TOF-MS spectrum of **1** in CH_2Cl_2/CH_3OH.

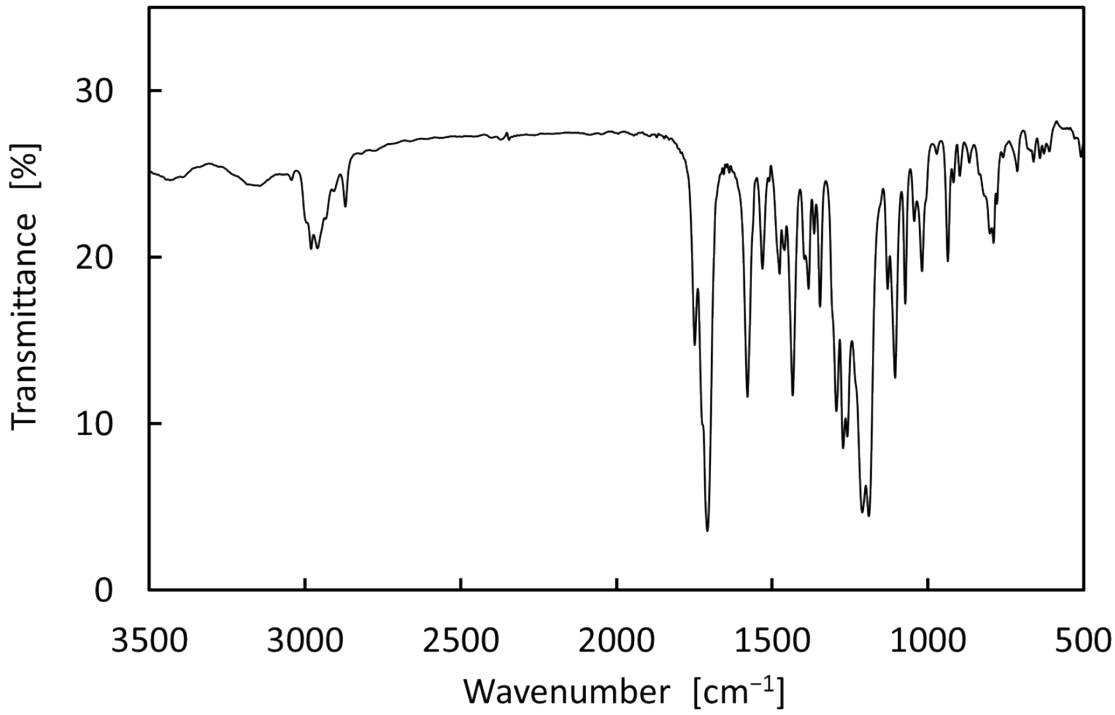


Fig S9. IR spectrum of **1** measured by a KBr method.

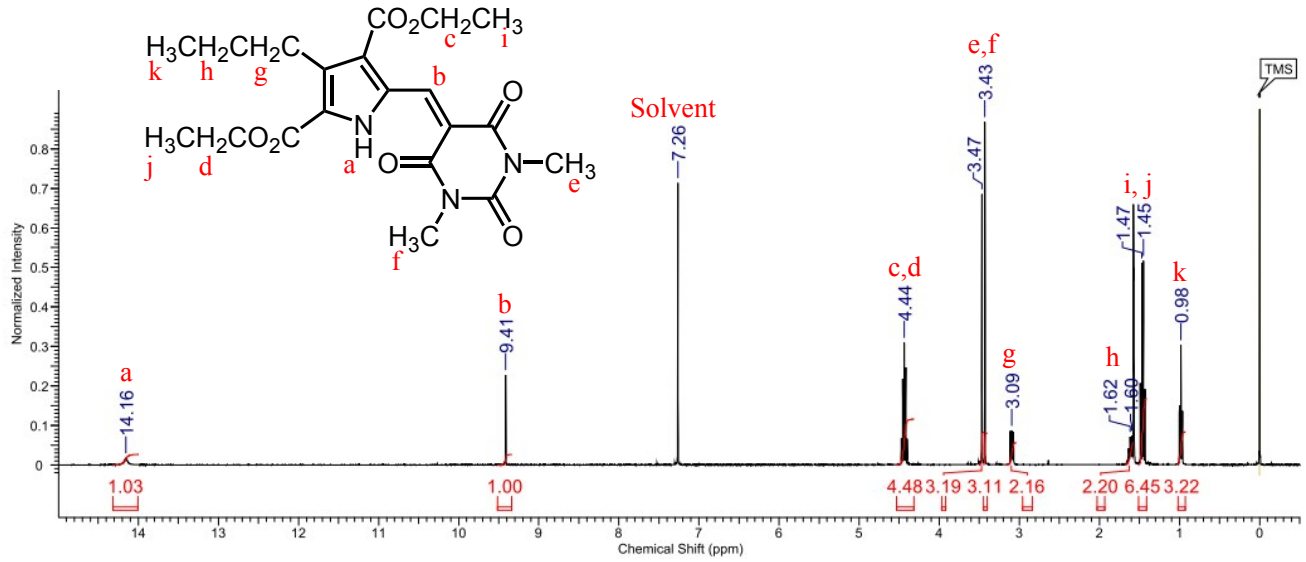
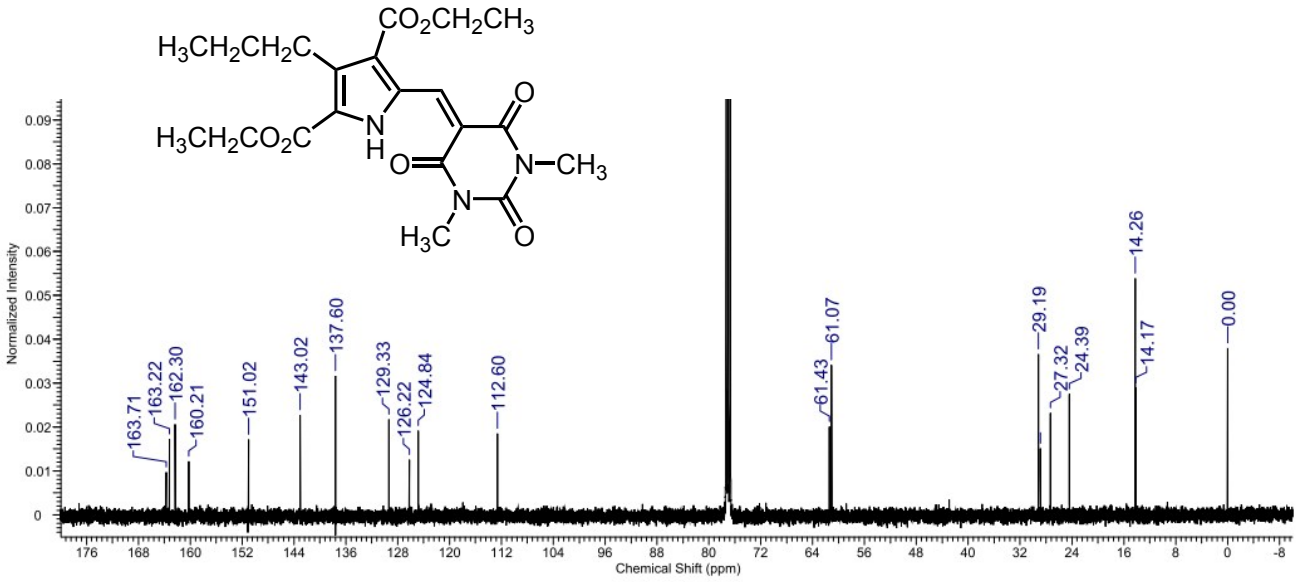
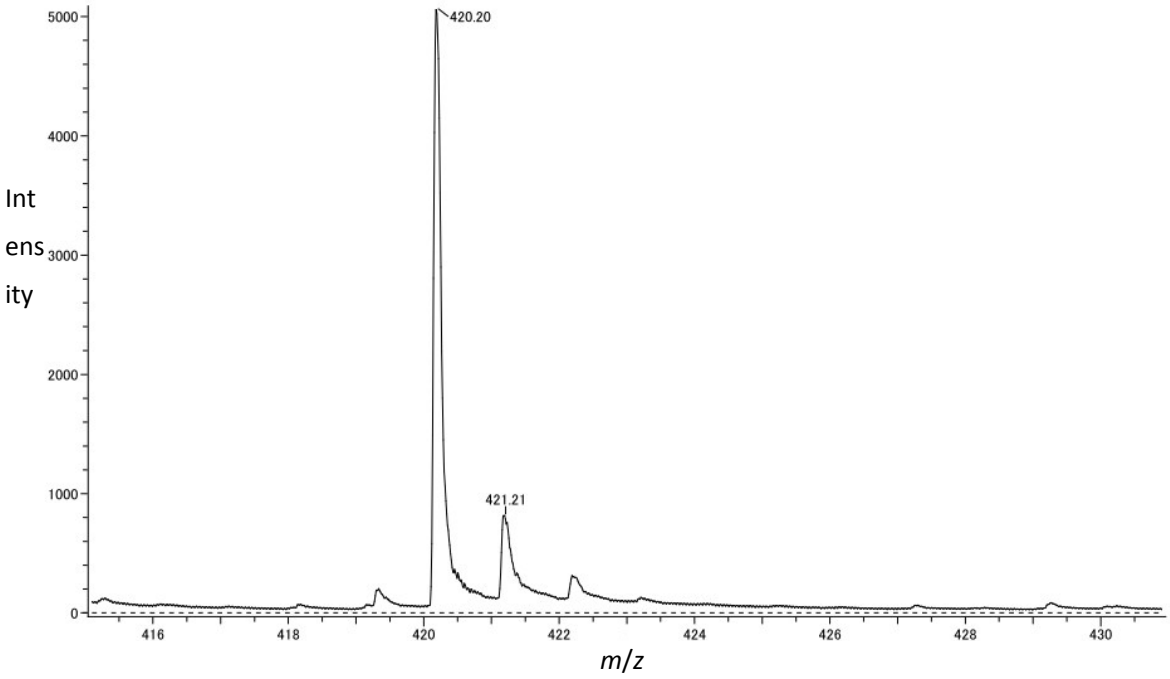


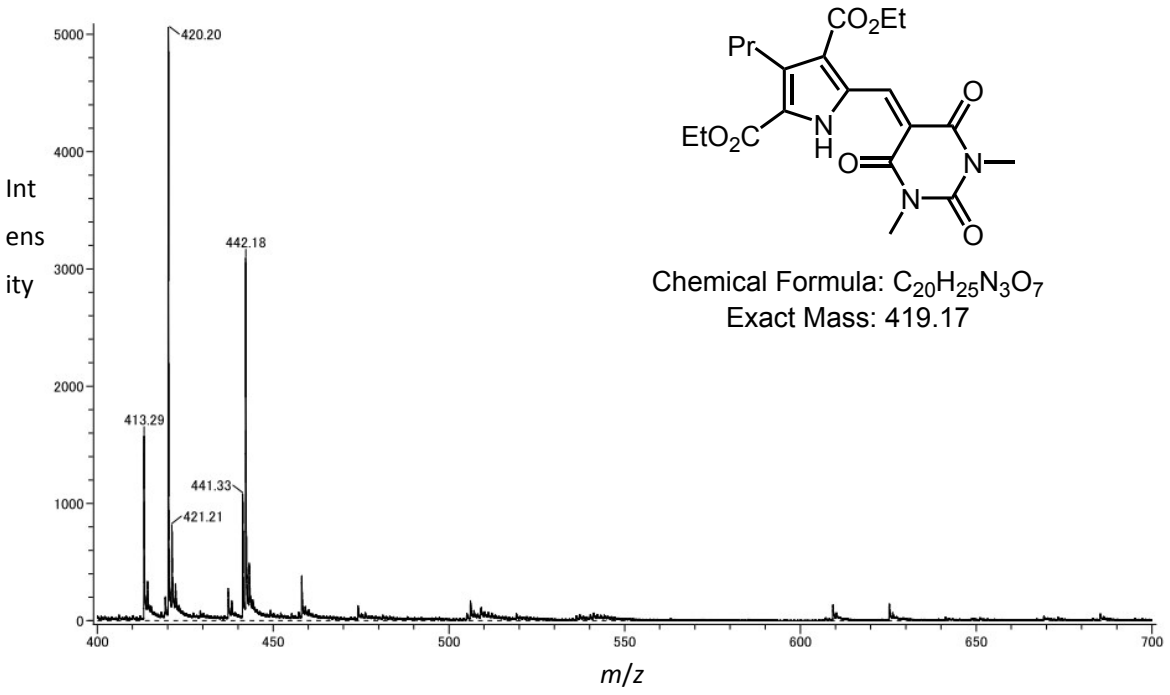
Fig S10. ^{1}H NMR spectrum of **2** in $CDCl_3$ at 25℃.



No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height	No.	(ppm)	(Hz)	Height
1	0.00	0.0	0.0380	5	27.32	2746.3	0.0232	9	61.43	6174.8	0.0201	13	129.33	13001.1	0.0217	17	160.21	16105.5	0.0122
2	14.17	1424.9	0.0289	6	28.85	2899.9	0.0151	10	112.60	11319.2	0.0185	14	137.60	13832.7	0.0316	18	162.30	16315.6	0.0206
3	14.26	1433.8	0.0539	7	29.19	2934.7	0.0366	11	124.84	12549.3	0.0192	15	143.02	14377.5	0.0228	19	163.22	16407.7	0.0173
4	24.39	2452.1	0.0276	8	61.07	6139.3	0.0342	12	126.22	12688.3	0.0126	16	151.02	15180.9	0.0171	20	163.71	16457.0	0.0097

Fig S11. ^{13}C NMR spectrum of **2** in $CDCl_3$ at 25℃.





Chemical Formula: $C_{20}H_{25}N_3O_7$
Exact Mass: 419.17

Fig S12. ESI-TOF-MS spectrum of **2** in CH_2Cl_2/CH_3OH.

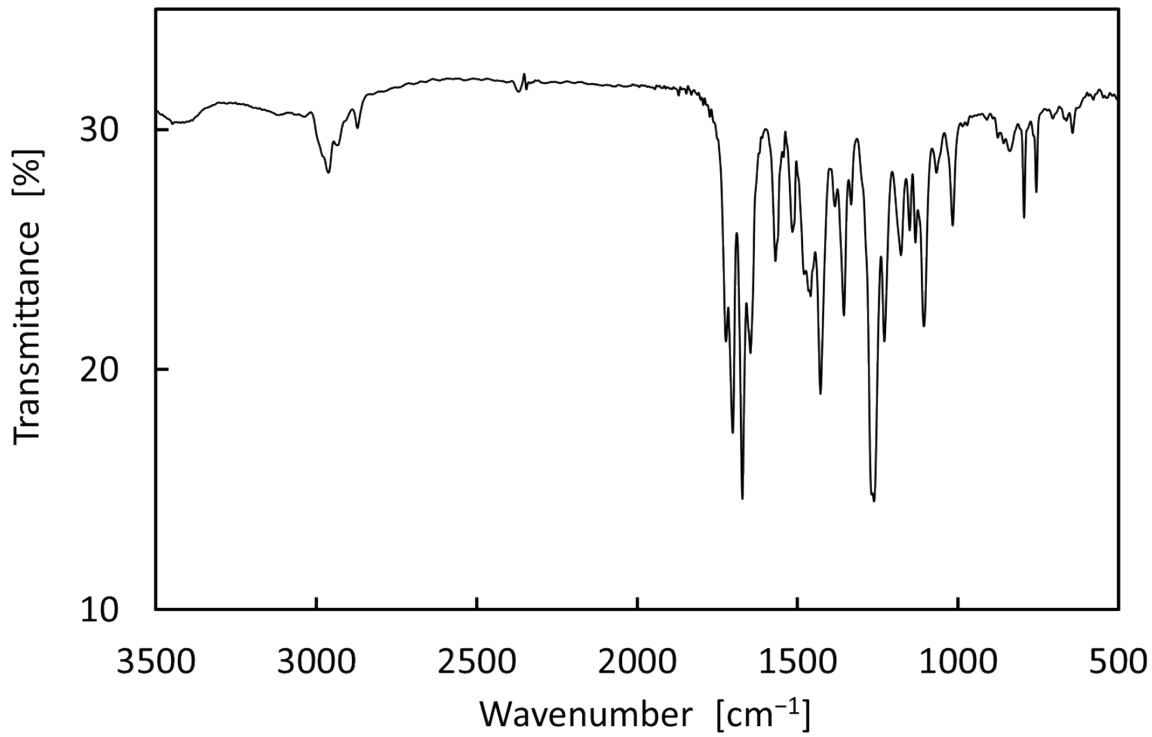


Fig S13. IR spectrum of **2** measured by a KBr method.

Table S4. Summary of the CHN elemental analysis of **1** and **2**.

Compounds		Weight [µg]	H [%]	C [%]	N [%]
1	Found[(a)]	1414.2	6.14	59.07	3.56
	Calculated	–	6.19	58.96	3.44
2	Found[(a)]	1355.1	5.89	56.98	9.86
	Calculated	–	6.01	57.27	10.02

(a) Recorded on a Yanaco CHN Corder MT-5 analyzer.

Aggregation-induced emission behavior in THF/water mixture

Stock solutions of **1** and **2** in THF with a concentration of 1.0×10^{-3} M were prepared. The aggregates were freshly prepared by adding water into the pyrrole solutions to make a total amount of 5 mL mixture. For example, the water fraction of 80% mixture including 1.0×10^{-4} M of a dye was prepared by 0.50 mL of the stock solution and diluted with 0.50 mL of THF followed by addition of 4.0 mL water. The fluorescence spectra were recorded by Hitachi F7000 spectrophotometer. Fluorescence and excitation slit widths were set to 5.0 nm and 10.0 nm, respectively. All spectra were recorded under 365 nm excitation wavelength.

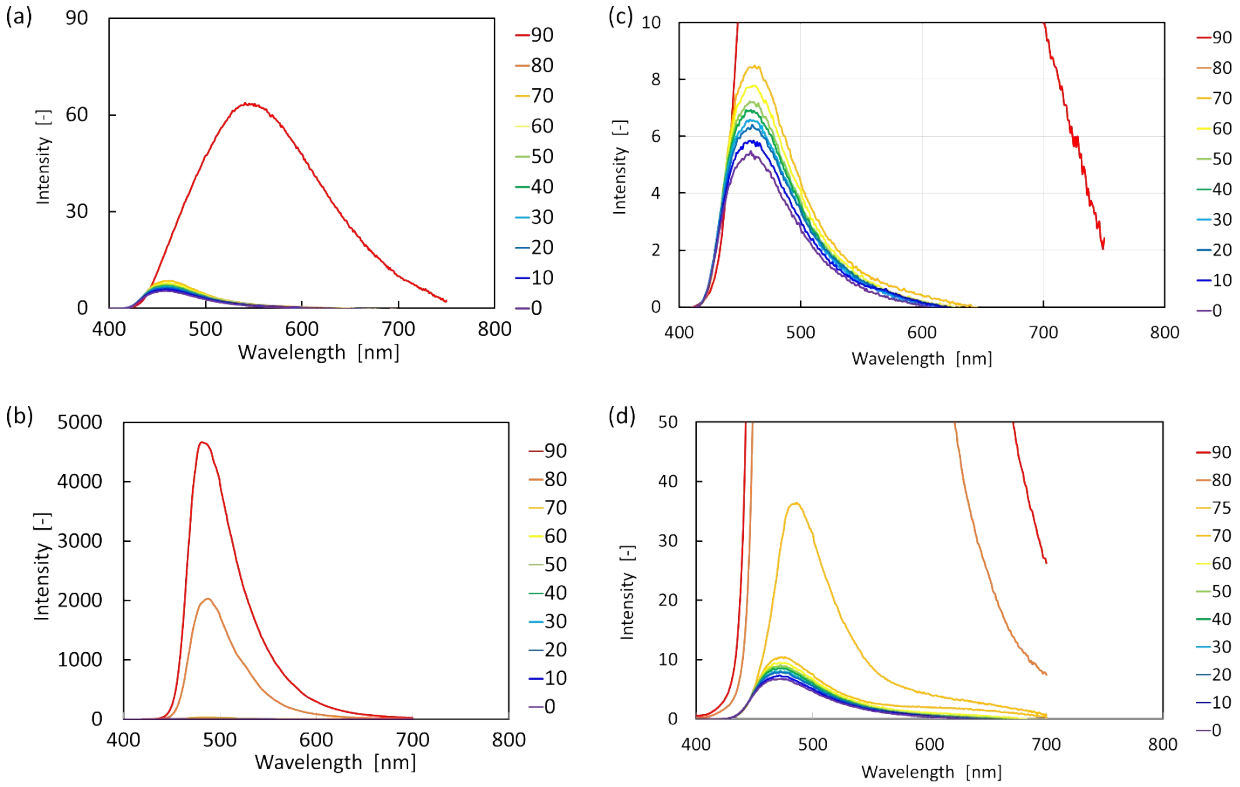
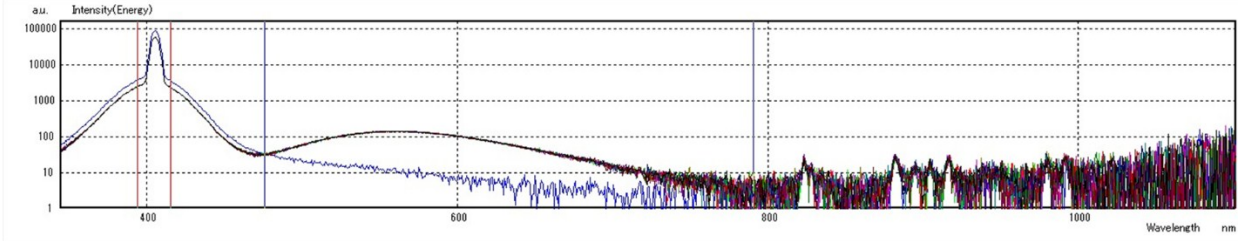


Fig S14. Photoluminescence spectral changes of (a) **1** and (b) **2** (1×10^{-4} M) based on the water fraction present in the THF solution. Photophysical spectral changes of (c) **1** and (d) **2** (1×10^{-4} M) based on the water fraction between 0 and 80%.

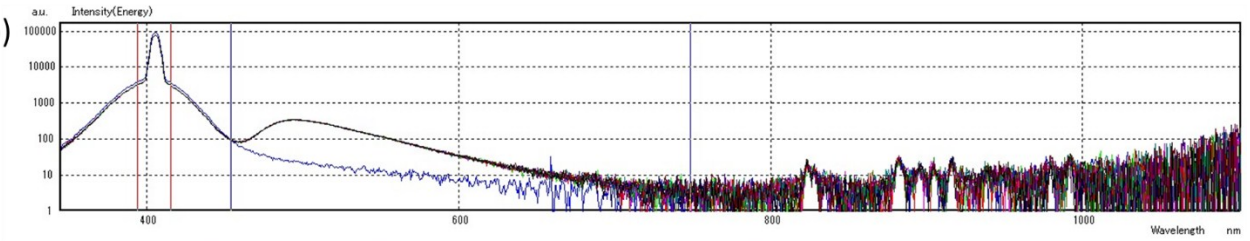
Absolute fluorescence quantum yield measurements for 1 and 2

(a)



N...	Cursor1-2: 393.97 - 415.2...	Cursor3-4: 475.74 - 790.5...	QuantumYield	Abs	Peak Wavele...	Peak Co...	Peak FW...	Peak Wavele...	Peak Co...	Peak FW...
1	251918480	---	---	---	404.60	93306.16	5.98	477.25	33.76	506.57
2	165479646	8446076	0.098	0.343	404.60	61479.80	5.97	563.03	146.01	115.05
3	165718604	8492103	0.099	0.342	404.60	61562.51	5.97	557.02	145.46	116.64
4	165630792	8372596	0.097	0.343	404.60	61501.30	5.97	560.77	146.99	113.55
5	165753748	8400735	0.097	0.342	404.60	61493.15	5.98	563.78	148.03	112.75
6	165671709	8457637	0.098	0.342	404.60	61585.25	5.97	556.27	145.79	115.73
7	165715659	8392426	0.097	0.342	404.60	61516.91	5.97	557.02	145.87	113.34
8	165712699	8389504	0.097	0.342	404.60	61572.69	5.97	560.02	144.88	115.18
9	165714458	8394711	0.097	0.342	404.60	61507.52	5.97	560.77	146.18	114.26
10	165832034	8372986	0.097	0.342	404.60	61539.88	5.97	556.27	148.04	113.29
11	165728698	8427332	0.098	0.342	404.60	61477.20	5.98	560.02	146.08	113.64

(b)



N...	Cursor1-2: 393.97 - 415.2...	Cursor3-4: 453.83 - 748.4...	QuantumYield	Abs	Peak Wavele...	Peak Co...	Peak FW...	Peak Wavele...	Peak Co...	Peak FW...
1	253610037	---	---	---	404.60	93823.57	5.99	453.83	88.80	467.73
2	212177160	10070946	0.243	0.163	404.60	78545.69	5.98	493.84	350.02	58.75
3	212336763	10064855	0.244	0.163	404.60	78567.75	5.99	494.60	347.19	59.93
4	212219667	10084267	0.244	0.163	404.60	78515.37	5.98	492.33	348.07	59.03
5	212244098	10022173	0.242	0.163	404.60	78491.15	5.99	493.84	346.33	59.24
6	212235635	10120894	0.245	0.163	404.60	78486.74	5.99	493.84	353.13	57.79
7	212240588	10108824	0.244	0.163	404.60	78476.90	5.99	493.09	345.08	59.99
8	212345291	10136814	0.246	0.163	404.60	78582.57	5.99	493.84	348.34	58.67
9	212187538	10107425	0.244	0.163	404.60	78532.11	5.99	493.09	347.77	59.61
10	212312027	10211932	0.247	0.163	404.60	78564.36	5.98	493.09	350.30	58.13
11	212266276	10067235	0.244	0.163	404.60	78498.06	5.99	494.60	347.11	59.98

Fig S15. Absolute quantum yield measurements of (a) **1** and (b) **2**.

Time-dependent density functional theory (TD-DFT) calculations for 1 and 2

Initial coordinates for **1**

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	10.3528	7.1517	7.5259
C	10.0589	8.5434	7.3545
C	9.0757	8.6099	6.2814
C	8.7777	7.2437	5.8598
C	7.8304	6.7811	4.8468
H	7.4655	7.475	4.3475
C	7.354	5.5261	4.464
C	7.8098	4.2021	5.0366
C	6.3159	5.4928	3.3502
C	5.6442	3.3228	4.2505
C	5.1812	1.963	3.6774
H	4.3148	2.0627	3.2758
H	5.134	1.3163	4.3856
H	5.8085	1.6652	3.0143
C	4.7397	3.8238	5.3863
H	5.0739	4.6621	5.7153
H	4.7336	3.1797	6.0979
H	3.8477	3.9452	5.0556
C	11.3061	6.4539	8.4716
C	12.2704	4.2634	8.9962
H	12.102	4.3938	9.9433
H	13.1889	4.5139	8.8127
C	12.0436	2.8154	8.6257
H	11.1225	2.5892	8.766
H	12.5981	2.2544	9.1728
H	12.2679	2.6838	7.7012
C	8.3825	9.8291	5.7135
C	8.3195	12.2675	5.717
H	8.3498	12.3813	4.7544
H	7.3925	12.2816	6.0027
C	9.0933	13.3308	6.394
H	9.0651	13.1915	7.3428
H	8.7114	14.1871	6.1845
H	10.004	13.3053	6.0927

C	10.7308	9.6821	8.1531
H	10.9138	9.369	9.0516
H	10.112	10.4259	8.2188
C	12.0658	10.1933	7.5142
H	12.7053	9.4649	7.4986
H	11.8955	10.4579	6.5965
C	12.6822	11.3934	8.2794
H	12.0912	12.1474	8.224
H	13.5296	11.6209	7.8899
H	12.8103	11.1544	9.2005
N	9.5826	6.4194	6.6355
H	9.601	5.5619	6.5706
O	8.8476	3.9963	5.7092
O	7.0258	3.1094	4.7428
O	6.041	6.4347	2.6061
O	5.6547	4.2787	3.1428
O	11.9677	6.9855	9.3674
O	11.3424	5.1056	8.1955
O	7.3831	9.8099	4.9846
O	8.9756	10.9857	6.1187

Initial coordinates for **2**

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

O	0.8615	1.1703	5.7247
O	5.8879	5.4566	7.3204
O	0.6344	5.3182	9.4842
O	-0.3549	3.712	8.2849
O	5.8804	4.0785	5.569
O	4.9588	1.0357	3.3342
O	1.647	-1.9247	2.5423
N	1.9803	3.1649	6.9891
H	1.3131	2.6263	6.7911
N	1.2642	-0.392	4.1582
N	3.3408	-0.5011	3.0078
C	1.9293	4.1348	7.9266
C	2.0399	-1.0043	3.1852
C	3.2073	3.1326	6.3891
C	3.0144	1.2168	4.6847

C	5.3422	4.5363	6.5465
C	3.9709	4.1578	7.0005
C	1.6594	0.7016	4.9165
C	3.6041	2.2446	5.3617
H	4.4964	2.4015	5.0744
C	0.6321	4.3452	8.5792
C	3.1786	4.79	7.9871
C	3.5587	5.8831	8.934
H	2.7393	6.3335	9.2605
H	4.1068	6.5544	8.4562
C	3.8488	0.5935	3.6497
C	-0.0751	-0.9407	4.3853
H	-0.7438	-0.3494	3.9803
H	-0.2412	-1.0087	5.3492
H	-0.1374	-1.8304	3.9799
C	4.3472	5.3376	10.1234
H	3.7709	4.7165	10.6375
H	5.1247	4.8245	9.7906
C	4.1758	-1.1662	1.9959
H	4.9984	-1.4949	2.4146
H	4.4028	-0.527	1.2879
H	3.6828	-1.9198	1.6085
C	-0.4502	6.7579	11.0353
H	-0.277	7.5654	10.5066
H	0.3202	6.5757	11.6134
H	-1.2482	6.8928	11.5861
C	7.1839	5.9744	6.8801
H	7.119	6.3312	5.958
H	7.8666	5.2574	6.8937
C	7.5503	7.067	7.8415
H	8.4033	7.4665	7.5718
H	7.6339	6.6934	8.7429
H	6.8513	7.7541	7.8355
C	-0.6685	5.598	10.1148
H	-0.9834	4.8088	10.623
H	-1.3443	5.8236	9.4284
C	4.8294	6.4249	11.0331
H	5.3677	7.0636	10.5219
H	5.3747	6.0352	11.748
H	4.0591	6.8877	11.4262

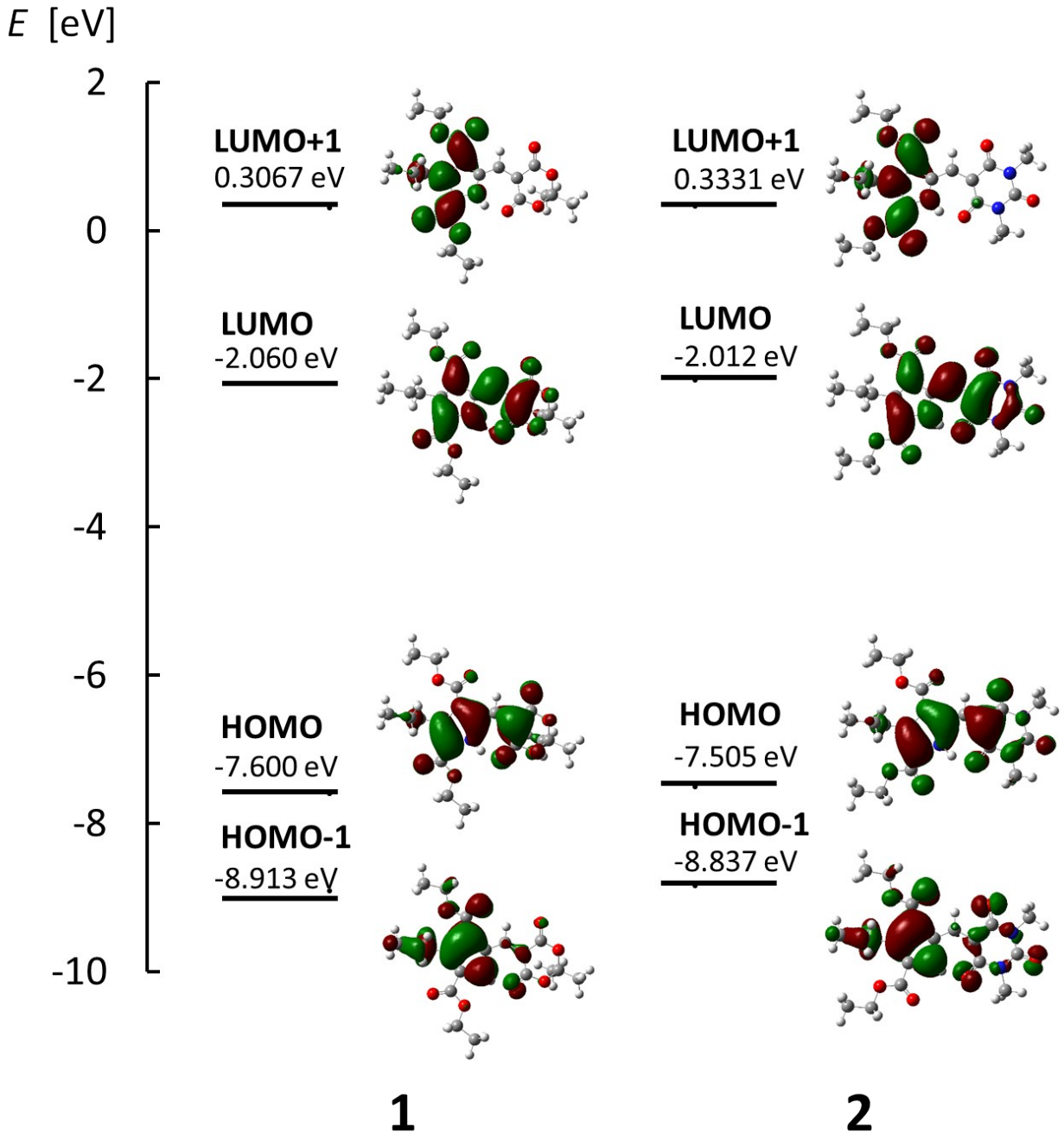


Fig S16. Calculated orbital energy diagrams of **1** and **2**.